Differentiability of the volume of a region enclosed by level sets

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Abstract

The level of a function f on $\mathbb{R}^n$ encloses a region. The volume of a region between two such levels depends on both levels. Fixing one of them the volume becomes a function of the remaining level. We show that if the function f is smooth, the volume function is again smooth for regular values of f. For critical values of f the volume function is only finitely differentiable. The initial motivation for this study comes from Radiotherapy, where such volume functions are used in an optimization process. Thus their differentiability properties become important.

1 Introduction

The volume of a set enclosed by two different level sets of a function $f : \mathbb{R}^n \to \mathbb{R}$ depends on both levels. Here we fix one level and the question we want to address is the differentiability of the volume as a function of the varying level for arbitrary dimension n. It will turn out that under mild conditions, among which smoothness of f, this function is again smooth for all regular values of f, but only finitely differentiable at critical values of f. Moreover we also consider f on a compact subset V of its domain and subsequently pose the same question for level sets restricted to V. Then we get a similar differentiability result when we also include the levels of f restricted to the boundary of V. In section 2 we will more precisely define the situation we consider and give precise statements of our results.

The initial motivation for this study comes from Radiotherapy. A patient is treated with ionizing radiation causing energy release per unit mass or volume inside the patient, which is called dose. The above mentioned function f represents this dose and the set V represents a patient's organ or a tumour region. The therapeutic outcome of Radiotherapy treatment not only depends on the dose on the tumour but also on the dose on healthy organs. Since it is usually hard to estimate the effect of dose in three dimensons, one reduces it for each tumour and organ to a so called *dose-volume histogram*, see [2]. In it one records for each dose value which fraction of the volume receives at least this dose. The resulting collection of dose-volume pairs is called the *cumulative* dose-volume histogram, which is closely related to the volume function introduced in the first paragraph. It is well established that the larger the fraction of the volume of a tumour receiving a prescribed dose, the larger the probability that the tumour is eradicated. For healthy organs and tissues the situation is less clear but some evidence exists that damage can be estimated from dose-volume histograms, see [2] and references therein.

In Radiotherapy treatment planning one tries to find an optimum for a sufficiently high dose on a tumour and a sufficiently low dose on healthy organs. The object function of this optimization process depends in particular on certain dose-volume pairs $(d, v(d))$ on the graph of the cumulative dose-volume histogram, see [5]. In the optimization process we have a family of dose functions and thus a family of dose-volume histograms, parametrized by the optimization variables. Anticipating the result on finite differentiability of the dose-volume histogram at a critical value of the dose function, we conclude that the object function is finitely differentiable at values of the optimization variables for which d is a critical value of the dose function. Because many numerical methods to solve such problems assume differentiability of the object function to some order, differentiability of the dose-volume function becomes important.

The remaining part of this article is organized as follows. In section 2 we give a summary of the results, preceded by definitions. In section 3 we sketch the idea of the proof and the results are proved in a series

of propositions. Some of the more elaborate computations are summarized in an appendix.

2 Statement of results

2.1 Definitions

Our main object is a smooth positive function f which is bounded and whose levelsets are compact. These properties are sufficient for our results, we do not claim necessity. We now define a function class for future reference.

Definition 1 *Let C be the class of functions $f : \mathbb{R}^n \to \mathbb{R}$ satisfying the following*

a) f is C^∞,

b) f is positive,

c) f is decreasing, that is for each $\varepsilon > 0$ there is a compact $K \subset \mathbb{R}^n$ such that for all $x \in \mathbb{R}^n \setminus K$, $f(x) < \varepsilon$.

We define the levelsets N_c of $f \in C$ and sets U_c enclosed by levels in a straightforward manner.

$$
\begin{aligned}
N_c &= \{x \in \mathbb{R}^n \mid f(x) = c\}, \\
U_c &= \{x \in \mathbb{R}^n \mid f(x) \geq c\}.
\end{aligned}
$$

We wish to study the study the differentiability of the volume $\mathrm{vol}_n(U_c)$ of U_c as a function of c. Here $\mathrm{vol}_n(A)$ is the standard volume (Lebesgue measure) in $\mathbb{R}^n$ of a measurable set $A \subset \mathbb{R}^n$

$$
\mathrm{vol}_n(A) = \int_A 1 \, dx.
$$

When we restrict f to a subset V of $\mathbb{R}^n$ we make similar definitions. To be more precise, let $V \subset \mathbb{R}^n$ be a compact, connected, n-dimensional C^∞-manifold with boundary ∂V which is a $(n-1)$-dimensional C^∞-manifold. The restriction of f to V will be denoted by $f|_V$. We define $V_c = U_c \cap V$ and the volume function we consider for this case is $\mathrm{vol}(V_c)$.

As already indicated in the Introduction, the function vol need not be continuous. Indeed, let f be constant on an open neighbourhood of V then it is easily seen that vol is similar, upon scaling and translation, to the Heaviside function. In order to avoid this and other degeneracies we assume the following non-degeneracy conditions on f, $f|_V$ and V.

Definition 2 *Non-degeneracy conditions.*

a) Critical points of f are non-degenerate, that is if x is a critical point of f then $\det(\mathit{Hess}\, u(x)) \neq 0$.

b) If x is a critical point of f then $x \notin \partial V$.

c) Critical points of $f|_V$ are non-degenerate.

d) f is fine, *that is if x and y are critical points and $x \neq y$ then $f(x) \neq f(y)$.*

e) $f|_V$ is fine.

Remarks

1. Conditions a, b and c are essential for our proofs. If one of them is not satisfied our standard forms, see section 3, of f and V are no longer valid. In order to proceed we would need higher order information about f and V. Moreover the critical point would not be stable under small perturbations. At the moment we are not interested in such a situation. Conditions d and e are for convenience only and can easily be dropped.

2. In principle, the sets U_h, V and V_h need not be connected. If one of them consists of several components, the construction in the following sections can be carried out for each component separately. Therefore without loss of generality we may as well assume connectedness.

3. In Radiotherapy one sometimes uses the so called *differential* dose-volume histogram, see [2]. However in general this is not a function. In terms of our function f it is in fact the image measure of the standard measure on $\mathbb{R}^3$ under f on $\mathbb{R}$, see [1]. Instead of studying the volume function via f as defined in this section one could also study the volume function via this measure. The present approach however seems to be simpler.

2.2 Results

In order to state the results we will make a distinction between regular values and critical values of $f|_V$. In case of a critical value of $f|_V$ we make a further distinction whether the critical point is in ∂V or not. Results for f and $f|_V$ are identical when the critical point is not in ∂V, therefore they are not stated separately. Our proofs are valid only for f in class C, see definition 1, satisfying the nondegeneracy conditions in definition 2.

The first theorem states that for all regular values of the function f, which means for almost all values by virtue of the nondegeneracy conditions, the volume function is a smooth function of the level.

Theorem 1 *Let $0 \in \mathbb{R}$ be a regular value of $f|_V$ then $\mathrm{vol}(V_h)$ is a smooth function of h at 0.*

The second and third theorem state that at a critical value the differentiability of the volume function is finite. The order of differentiability depends on the dimension of the domain of f. The nature of the discontinuity depends on the Morse index of f at the critical point. Together with the proofs we give details about the discontinuity in the next section.

Theorem 2 *Let $0 \in \mathbb{R}$ be a critical value of $f|_V$ and let $0 \notin \partial V$ be the critical point. Then the $\lceil \frac{n}{2} \rceil$-th derivative of $\mathrm{vol}(V_h)$ is discontinuous at $h = 0$, all lower order derivatives are continuous.*

Theorem 3 *Let $0 \in \mathbb{R}$ be a critical value of $f|_{\partial V}$ and let $0 \in \partial V$ be the critical point. Then the $\lceil \frac{n+1}{2} \rceil$-th derivative of $\mathrm{vol}(V_h)$ is discontinuous at $h = 0$, all lower order derivatives are continuous.*

In a Radiotherapy setting, which originally motivated this study, the dimension of the domain of f, representing dose, is 3. This means that at a critical point of dose, the volume function is not even twice continuously differentiable. As mentioned in the introduction one aimes at finding an optimum for a suffiently high dose on the tumour and a sufficiently low dose on healthy organs. The objective function in this optimization process depends on the volume function. Many iterative optimization methods use a quasi-Newton method in the background and thus require differentiability to second order. Such a method is not guaranteed to be well behaved near a critical value of dose.

3 Proof of results

We will work in the class of C^∞-functions. This class is closed under the action of the group of C^∞-transformations. Therefore we have the notion of C^∞-equivalence of functions. We use this to put the function at hand into a suitable standard form. In general however, this standard form is only valid locally in a small open ball.

Now our aim is to compute the volume of the set enclosed by two levelsets of a function, which is a global rather than a local problem. A natural way to look at this set is by "sweeping out" using the gradient flow of the function. Using compactness we can then turn this into a local problem considering flow boxes of the gradient flow starting in small subsets, here we take $(n-1)$-simplices, of the levelset corresponding to the lower level and ending in the levelset corresponding to the higher level. By a suitable C^∞-transformation we turn each flow box into a Cartesian product of a $(n-1)$-simplex and an interval. This greatly simplifies finding the volume of the enclosed set and its dependence on the level.

A complication in this procedure is that a general C^∞-transformation does not map a pair $(f, \mathrm{grad} f)$ into a new pair $(g, \mathrm{grad} g)$. In order to achieve the latter, the transformation would have to preserve the inner product which is used to define grad. For our purposes this is too stringent a restriction. Another

reason not to use the gradient flow is the following. We also wish to consider the set enclosed by levelsets restricted to a set V. The gradient flow is not necessarily tangent to ∂V, thus the flow box we construct might not be restricted to V. Instead we use the flow of a C^∞-vectorfield which is only transversal to the levelsets and tangent to ∂V if necessary. These properties are preserved by a general C^∞-transformation.

The tansformations we apply to a flow box do not in general preserve its volume. Here, however, we are only interested in the h dependence of this volume, not in its numerical value. Therefore we may apply affine transformations without any further considerations. With other transformations we have to be more careful and we will take them into account at the appropriate places.

Let us sketch the steps in the proofs of theorems 1, 2 and 3. If 0 is a regular value of f, all points in V_h are regular for h small enough. We first construct a finite number of boxes B_i covering V_h using a triangulation of N_0 and a regular flow from N_0 to N_h. Assuming the boxes B_i are small enough we put each of them in standard form by several local C^∞-transformations. The first transformation parallellizes the flow from N_0 to N_h. The second transformation is linear and preserves the parallellity of the flow but makes it perpendicular to N_0 at 0 and parallel to the last basis vector e_n of $\mathbb{R}^n$. The third transform takes f into a local standard form preserving all of the previous. The result is that B_i is transformed to the Cartesian product of a simplex in N_0 and the interval $[0, h]$. The conclusion is that the volume of B_i is a smooth function of h.

If 0 is a critical value of f we use the fact that 0 is the only critical point on N_0. We construct one special box B_0 containing 0 and away from 0 we use the same construction as above. Differentiability is then determined by $\text{vol}(B_0)$. Again we use a transformation that takes f into standard form, but now at the critical point.

The main part of the proof of theorem 1 is the construction of the boxes and putting them into a standard form. In the proofs of the other theorems the emphasis is on computing the volume of box B_0.

Where necessary we assume the existence of a standard basis and a standard inner product.

3.1 Proof of theorem 1

Proposition 4 *Let 0 be a regular value of f, then for sufficiently small $h > 0$ there exists a finite collection of sets B_i with $i \in I \subset \mathbb{N}$ satisfying*

a) $V_h = \cup_{i \in I} B_i$
b) $\text{vol}_n(V_h) = \sum_{i \in I} \text{vol}_n(B_i)$.

Proof of proposition 4.
Construction. If 0 is a regular value of f then N_0 is a smooth manifold. The non-degeneracy conditions imply that critical values of f are isolated, therefore an $h_0 > 0$ exists such that all $h \in [0, h_0]$ are regular values. Then all N_h are diffeomorphic to N_0, see [3]. First we assume that N_0 does not intersect the boundary ∂V of V. Since N_0 is a compact C^∞-manifold it allows a finite triangulation with $(n-1)$-simplices $\sigma_{i,n-1}$ and $i \in I \subset \mathbb{N}$, see [4]. One of the properties of a triangulation is that for $i \neq j$ either $\sigma_{i,n-1} \cap \sigma_{j,n-1} = \varnothing$ or $\sigma_{i,n-1} \cap \sigma_{j,n-1} = \sigma_{k,n-2}$ for some k and $(n-2)$-simplex $\sigma_{k,n-2}$. Let X be a C^∞-vector field transversal to N_h for all $h \in [0, h_0]$. More precisely we impose the condition that there is an $\varepsilon > 0$ such that $|\langle n_h(x), X(x)\rangle| > \varepsilon$ for all $x \in N_h$ and $h \in [0, h_0]$, where $n_h(x)$ is a unit normal to N_h at x. Such a vectorfield exists, for example $\text{grad} f$. If N_0 intersects ∂V then the non-degeneracy conditions imply that the intersection of N_h and ∂V is transverse for all $h \in [0, h_0]$. We restrict to $N_0 \cap V$ which is still a compact C^∞-manifold. Now we impose one more condition on the vector field X namely that it is tangent to $\partial V \cap V_{h_0}$. Let $\Phi \in \text{Diff}(\mathbb{R}^n)$ be the flow of X with $\Phi(x, 0) = x$. Finally we define

$$B_i = \{\Phi(x,t) \mid x \in \sigma_{i,n-1}, t \in [0,T]\} \cap V_h.$$

Proof of $V_h = \cup_{i \in I} B_i$. Clearly $\cup_{i \in I} B_i \subset V_h$. Suppose $x \in V_h$, then $\frac{d}{dt} f(\Phi(x,t))$ is strictly increasing or decreasing since $|\langle n_h(x), X(x)\rangle| > \varepsilon$. In either case a finite t_0 exists such that $f(\Phi(x, t_0)) = 0$. This means $x_0 = \Phi(x, t_0) \in N_0$, therefore an i exists such that $x_0 \in \sigma_{i,n-1}$ which implies $x \in B_i$. Compactness of V_h guarantees that a $T > 0$ exists such that for all $x \in V_h$, $|t_0| \in [0, T]$. The conclusion is that $V_h = \cup_{i \in I} B_i$.
Proof of $\text{vol}_n(V_h) = \sum_{i \in I} \text{vol}_n(B_i)$. It suffices to show that for $i \neq j$, $\text{vol}_n(B_i \cap B_j) = 0$. Suppose

$B_i \cap B_j \neq \varnothing$ and $x \in B_i \cap B_j$, then there is a t_0 such that $x_0 = \Phi(x, t_0) \in N_0$. By definition $\Phi(x,t) \in B_i \cap B_j$ therefore $x_0 \in B_i \cap B_j$ which means $x_0 \in \sigma_{i,n-1} \cap \sigma_{j,n-1} = \sigma_{k,n-2}$. From this we conclude $B_i \cap B_j = \{\Phi(x,t) \mid x \in \sigma_{k,n-2}, t \in [0,T]\} \cap V_h$. But then $\dim(B_i \cap B_j) = n-1$ and therefore $\mathrm{vol}_n(B_i \cap B_j) = 0$. ■

The next step is to put the boxes B_i of proposition 4 into a standard form. To do this we also need a local standard form of the function f.

Proposition 5 *Let f be a function as in definition 1, satisfying the non-degeneracy conditions in definition 2 and $f(0) = 0$. We distinguish three different cases:*

a) 0 is a regular point of f,

b) 0 is a critical point of f,

c) 0 is a critical point of $f|_{\partial V}$.

Then an open neighbourhood $\mathcal{O}$ of 0 and a diffeomorphism Φ exist such that $F = \Phi_* f$ takes one of the forms:

a) $F(\xi, \eta) = \eta$, with $(\xi, \eta) \in (\mathbb{R}^{n-1} \times \mathbb{R}) \cap \mathcal{O}$,

b) $F(\xi, \eta) = \sum_{i=1}^p \xi_i^2 - \sum_{i=1}^p \eta_i^2$, with $(\xi, \eta) \in (\mathbb{R}^p \times \mathbb{R}^q) \cap \mathcal{O}$ and $p + q = n$,

c) $F(\xi, \eta, \zeta) = \zeta + \sum_{i=1}^p \xi_i^2 - \sum_{i=1}^p \eta_i^2$ and ∂V is given by $\zeta = 0$ with $(\xi, \eta, \zeta) \in (\mathbb{R}^p \times \mathbb{R}^q \times \mathbb{R}) \cap \mathcal{O}$ and $p + q = n - 1$.

Remarks

1. Case b) of proposition 5 is called the Morse lemma. A critical point in this case has *Morse index* q, but some times it is more convenient say it has *Morse type* (p, q).

2. Due to non-degenracy condition 2, 0 is a critical point of $f|_{\partial V}$ as soon as 0 is a critical point of $f|_V$.

In the proof of 5 we will need a lemma which we only state here, for a proof see [3].

Lemma 6 *Let f be a C^∞ function on a convex neighbourhood $\mathcal{O} \subset \mathbb{R}^n$ of 0 with $f(0) = 0$. Then $f(x) = \sum_{i=1}^n x_i f_i(x)$ for certain C^∞ functions f_i with $f_i(0) = \frac{\partial}{\partial x_i} f(0)$.*

Proof of proposition 5.

a) Since 0 is a regular point of f there is a nonzero vector a such that $\mathrm{grad} f(0) = a$. After an orthogonal transformation we may assume that with respect to coordinates $(x, y) \in \mathbb{R}^{n-1} \times \mathbb{R}$ we have $\mathrm{grad} f(0, 0) = (0, |a|)$. Now we define new coordinates by the diffeomorphism $\Phi : (x, y) \mapsto (x, f(x, y))$, then $F = \Phi_* f$ takes the desired form.

b) See [3].

c) If 0 is a critical point of f_V, the the tangent spaces of N_0 and V at 0 coincide. By the non-degeneracy conditions 0 is a regular point of f. Using the arguments of case a) we assume that we already transformed to coordinates $(x, y) \in \mathbb{R}^{n-1} \times \mathbb{R}$ such that $\mathrm{grad} f(0, 0) = (0, |a|)$. Furthermore we made the assumption that ∂V is a smooth manifold, so at least locally it is the level set of a smooth function g. Now we apply part a) to bring g into standard form, then on new coordinates $(u, v) \in \mathbb{R}^{n-1} \times \mathbb{R}$, ∂V is locally given by $v = 0$. After scaling in the v direction the function f satisfies: $f(0, 0) = 0$, $\frac{\partial}{\partial u_i} f(0, 0) = 0$ for $i \in \{1, \ldots, n-1\}$ and $\frac{\partial}{\partial v} f(0, 0) = 1$. The remainder of the proof is only a slight adaption of the proof in [3] for case b), but included here for the sake of completeness. Applying lemma 6 to f and its partial derivatives we get

$$f(u, v) = \sum_{i,j<n} u_i u_j \alpha_{ij}(u, v) + v f_n(u, v)$$

where α_{ij} and f_n are smooth functions and $f_n(0,0) = 1$. As a first step we apply the transformation $(u, v) \mapsto (u, vf_n(u, v)) = (u, z)$, preserving the standard form of g since $f_n(0,0) \neq 0$. Then f takes the form

$$f(u, z) = \sum_{i,j<n} u_i u_j \alpha_{ij}(u, z) + z$$

with new functions α_{ij}. From now on we only apply transformations of the form $(u, z) \mapsto (\phi(u, z), z)$ and we proceed by induction. We assume that

$$f(u, z) = \pm u_1^2 \cdots \pm u_{k-1}^2 + \sum_{i,j=k}^{n-1} u_i u_j \alpha_{ij}(u, z) + z$$

for a certain $k > 0$. Now let $\hat{u}_i = u_i$ for $i \neq k$ and $\hat{z} = z$ and

$$\hat{u}_k = \sqrt{\alpha_{kk}(u, z)}(u_k + \sum_{i=k+1}^{n-1} u_i \alpha_{ik}(u, z)/\alpha_{kk}(u, z))$$

In order to define $\hat{u}_k$ it may be necessary to permute the rows of α_{ij} so that $\alpha_{kk}(u, z) \neq 0$. Such a permutation exists because $\det(\text{Hess}f(0, 0)) \neq 0$ which means there is at least one $i \in \{k, \ldots, n-1\}$ such that $\alpha_{ik}(0,0) \neq 0$. Then by continuity there is a neighbourhood of $(0,0)$ such that $\alpha_{ik}(u, z) \neq 0$. This means that in each induction step the neighbourhood on which our result holds might shrink. Since we only need a finitie number of steps this does not cause any problems. Dropping the hats we get in new coordinates

$$f(u, z) = \pm u_1^2 \cdots \pm u_k^2 + \sum_{i,j=k+1}^{n-1} u_i u_j \alpha_{ij}(u, z) + z$$

Renaming the variables we arrive at the desired form of $F = \Phi_* f$, where Φ is the composition of the transformations in each induction step. ■

Proposition 7 *Let $\{B_i\}_{i\in I}$ be a collection of boxes as in proposition 4. Let x be a point in the interior of $\sigma_{i,n-1}$ for some $i \in I$, without loss of generality we assume that $x = 0$. Then a diffeomorphism Φ exists such that*

$$\text{vol}_n(B_i) = \int_{B_i} 1\, dx = \int_0^h \left[\int_{\sigma_{i,n-1}} J_\Phi \, d\xi \right] d\eta,$$

where J_Φ is the Jacobian of Φ. Moreover $\text{vol}_n(B_i)$ is a smooth function of h.

Proof of proposition 7. The vector field in the construction of box B_i has no stationary point therefore it can be parallellized by a diffeomorphism Φ_1, see [4]. The next two transformations preserve parallellity because they are linear. By a linear diffeomorphism Φ_2 we can arrange that X is perpendicular to N_0 in 0. By another linear diffeomorphism Φ_3 we rotate such that X is parallel to the last basis vector of $\mathbb{R}^n$. The last diffeomorphism $\Phi_4 : (x, y) \mapsto (x, f(x, y))$ takes the function f into local standard form, see proposition 5. Since Φ_4 is a position dependent shift in the direction of the vectorfield, parallellity is again preserved. However the parametrization of the integral curves will change in general. Then $\Phi = \Phi_4 \circ \Phi_3 \circ \Phi_2 \circ \Phi_1$ is again a diffeomorphism and on new coordinates (ξ, η) we have $B_i = \sigma_{i,n-1} \times [0, h]$. Since J_Φ is a smooth function and $\text{vol}_n(B_i)$ depends on h only via the upper limit of the outer integral, $\text{vol}_n(B_i)$ is a smooth function of h. ■

Using the previous propositions we are able to prove theorem 1.

Proof of theorem 1. Construct boxes B_i as in proposition 4. Then by the same proposition $\text{vol}_n(V_h) = \sum_{i\in I} \text{vol}_n(B_i)$. In the latter $\text{vol}_n(B_i)$ is a smooth function of h by proposition 7. The finite number of boxes guarantees that also $\text{vol}_n(V_h)$ is a smooth function of h. ■

3.2 Proof of theorem 2

In the previous section all points were regular points of f. Here too points will be regular except the point 0 which now is a critical point. Therefore we will use the same construction of boxes as in the previous section. Only the box B_0 containing 0 will be treated differently. This means that differentiability in this situation is determined by $\mathrm{vol}_n(B_0)$.

A critical point with Morse index 0 is a minimum of f. If the Morse index is n the critical point is a maximum of f. Differentiability for minima and maxima is very similar so we only state a result for one of them. A critical point with Morse index q where $0 < q < n$ is called a saddle.

Proposition 8 *Let* 0 *be a non-degenerate critical point of* f *with Morse index* 0*, so* 0 *is a local minimum. Then the* $\lceil \frac{n}{2} \rceil$*-th derivative of* $\mathrm{vol}(V_h)$ *is not continuous at* $h = 0$*, all lower order derivatives are continuous.*

Proof of proposition 8. Let $h \geq 0$, then 0 is the minimal value of f so V_{-h} is empty. The level set N_0 only contains 0. Using the neighbourhood $\mathcal{O}$ of proposition 5 on which f takes its standard form we compute $\mathrm{vol}_n(V_h)$ using polar coordinates (r, φ), then that $u(r, \varphi) = r^2$. Here we assume that h is small enough so that $V_h \subset \mathcal{O}$. The Jacobian of the transformation Φ in proposition 5 will be denoted by J_Φ and the Jacobian of changing to polar coordinates by $r^{n-1} g_n(\varphi)$. Since Φ is non-singular and C^∞ we can split $J_\Phi = c + K_\Phi$ where $c \neq 0$ and both J_Φ and K_Φ are C^∞. Then we have

$$\mathrm{vol}_n(V_h) = \int_{V_h} 1\, dx = \int_{V_h} J_\Phi\, d\xi = c \int \int_0^{\sqrt{h}} r^{n-1}\, dr\, g_n(\varphi)\, d\varphi + \int_{V_h} K_\Phi\, d\xi.$$

For a non-differentiability result it is enough to consider the first integral in the last expression, since this integral contains the lowest order terms in h and we are interested in $h \to 0$ only. Let a_n be the “area” of S^{n-1} then

$$c \int \int_0^{\sqrt{h}} r^{n-1}\, dr\, g_n(\varphi)\, d\varphi = c\, a_n \int_0^{\sqrt{h}} r^{n-1}\, dr = \frac{c a_n}{n} h^{n/2}.$$

Thus we obtain the result that the $\lceil \frac{n}{2} \rceil$-th derivative is discontinuous at $h = 0$. ■

Proposition 9 *Let* 0 *be a non-degenerate critical point of* f*. Assume the Morse type of* 0 *is* (p, q) *with* $p \neq 0$ *and* $q \neq 0$*. Then the* $\lceil \frac{n}{2} \rceil$*-th derivative of* $\mathrm{vol}(V_h)$ *is discontinuous at* $h = 0$*. For both* p *and* q *even the discontinuity is a jump, for* p *and* q *odd it is a log-like singularity and for* $p + q$ *odd it is a root-like singularity. All lower order derivatives are continuous.*

Proof of proposition 9. Let h_0 be small enough so that 0 is the only critical point of f in V_{h_0}. Furthermore let $\mathcal{O}$ be a neighbourhood as in proposition 5 such that f can be put into standard form c). Changing to cylinder coordinates (r, φ, s, ψ) we may assume that $f(r, \varphi, s, \psi) = r^2 - s^2$. Then an $\varepsilon > 0$ exists such that $B = \{(r, \varphi, s, \psi) \in \mathbb{R} \times S^{p-1} \times \mathbb{R} \times S^{q-1} \mid r + s \leq \varepsilon\}$ is a subset of $\mathcal{O}$. The intersection of ∂B and N_0 is transversal so again taking h_0 small enough we may assume that ∂B transversally intersects N_h for all $h \in [0, h_0]$. Then $V_h \setminus B$ is a compact C^∞-manifold (with boundary) so we can apply the construction of boxes as in proposition 4. Where we have to impose the additional condition that the vector field X is tangent to the boundary ∂B of B. By proposition 7 $\sum_{i \in I} \mathrm{vol}_n(B_i)$ is a smooth function of h. If we now set $B_0 = B \cap V_h$ then $\mathrm{vol}_n(V_h) = \sum_{i \in I} \mathrm{vol}_n(B_i) + \mathrm{vol}_n(B_0)$. Thus differentiability of $\mathrm{vol}_n(V_h)$ is determined by the differentiability of $\mathrm{vol}_n(B_0)$.

The Jacobian of the transformation Φ in proposition 5 will be denoted by J_Φ and the Jacobian of changing to polar coordinates by $r^{p-1} s^{q-1} g_p(\varphi) g_q(\psi)$. The last transformation we apply is a scaling so that B is bounded by $r = 0$, $s = 0$ and $r + s = 1$. Then we get

$$\mathrm{vol}_n(B_0) = \int_{B_0} 1\, dx = \int_{B_0} J_\Phi\, d\xi\, d\eta = c \int_{B_0} 1\, d\xi\, d\eta + \int_{B_0} K_\Phi\, d\xi\, d\eta.$$

For our result we only need to compute the first integral in the last expression, using the same arguments as in the proof of proposition 8. The actual computation can be found in appendix A.1. From lemma 12 in the same appendix the result on differentiability follows. ■

Proof of theorem 2. The proof follows from propositions 8 and 9. ■

3.3 Proof of theorem 3

In this section 0 is a critical point of $f|_{\partial V}$, but all other points are regular. First we consider a critical point which is a minimum of $f|_{\partial V}$. Since for a maximum we get the same result we do not state it seperately.

Proposition 10 *Let 0 be a critical point of $f|_{\partial V}$. Assume the Morse type is $(n-1,0)$ with $n>1$. Then the $\lceil\frac{n+1}{2}\rceil$-st derivative of $\mathrm{vol}(V_h)$ is not continuous at $h=0$, all lower order derivatives are continuous.*

Proof of proposition 10. The proof is very similar to that of proposition 8 therefore we will only indicate the essential differences. On a neighbourhood $\mathcal{O}$ of 0 such that f can be put into standard form c) of proposition 5 we take cylinder coordinates $(r,\varphi,\zeta)\in\mathbb{R}\times\mathbb{R}^{n-2}\times\mathbb{R}$. Then locally $f(r,\varphi,\zeta)=r^2+\zeta$ and ∂V is given by $\zeta=0$. Splitting the Jacobian as in proposition 8 we obtain

$$\mathrm{vol}_n(V_h)=\int_{V_h}1\,dx=\int_{V_h}J_\Phi\,d\xi=c\int\int_0^{\sqrt{h}}\int_0^{h-r^2}r^{n-2}\,d\zeta\,dr\,g_{n-1}(\varphi)\,d\varphi+\int_{V_h}K_\Phi\,d\xi.$$

Only evaluating the first integral (cf. proof of proposition 8) we get

$$c\int\int_0^{\sqrt{h}}\int_0^{h-r^2}r^{n-2}\,d\zeta\,dr\,g_{n-1}(\varphi)\,d\varphi=2c\frac{a_{n-1}}{n^2-1}h^{(n+1)/2}.$$

Thus we obtain the result that the $\lceil\frac{n+1}{2}\rceil$-st derivative is discontinuous at $h=0$. ■

Next we turn our attention to saddle points of $f|_{\partial V}$.

Proposition 11 *Let 0 be a non-degenerate critical point of $f|_{\partial V}$. Assume the Morse type of 0 is (p,q) with $p\neq 0$, $q\neq 0$ and $p+q=n-1$. Then the $\lceil\frac{n+1}{2}\rceil$-st derivative of $\mathrm{vol}(V_h)$ is not continuous at $h=0$. For both p and q even the discontinuity is a jump, for p and q odd it is a log-like singularity and for $p+q$ odd it is a root-like singularity. All lower order derivatives are continuous.*

Proof of proposition 11. We proceed along the lines of the proof of proposition 9 again indicating the main differences only. Let $\mathcal{O}$ be a neighbourhood of 0 such that f can be transformed to standard form c) of proposition 5. Taking cylinder coordinates $(r,\varphi,s,\psi,q\zeta)$ we may assume that $f(r,\varphi,s,\psi,\zeta)=r^2-s^2+\zeta$. Then an $\varepsilon>0$ exists such that $B=\{(r,\varphi,s,\psi,\zeta)\in\mathbb{R}\times S^{p-1}\times\mathbb{R}\times S^{q-1}\times\mathbb{R}\mid r+s\leq\varepsilon,\ 0\leq\zeta\leq\varepsilon\}$ is a subset of $\mathcal{O}$. Once again taking h_0 small enough we may assume that ∂B transversally intersects N_h for all $h\in[0,h_0]$. Then $V_h\setminus B$ is a compact C^∞-manifold (with boundary) so here too we can apply the construction of boxes as in proposition 4 with the additional condition that the vector field X is tangent to ∂B. We set $B_0=B\cap V_h$ then $\mathrm{vol}_n(V_h)=\sum_{i\in I}\mathrm{vol}_n(B_i)+\mathrm{vol}_n(B_0)$. Now differentiability of $\mathrm{vol}_n(V_h)$ is determined by the differentiability of $\mathrm{vol}_n(B_0)$. Splitting the Jacobian as in proposition 9 we get

$$\mathrm{vol}_n(B_0)=\int_{B_0}1\,dx=\int_{B_0}J_\Phi\,d\xi\,d\eta\,d\zeta=c\int_{B_0}1\,d\xi\,d\eta\,d\zeta+\int_{B_0}K_\Phi\,d\xi\,d\eta\,d\zeta.$$

We only compute the first integral in the last expression (cf. proof of proposition 8). For the actual computation see appendix A.2. From lemma 13 in the same appendix the result on differentiability follows. ■

Proof of theorem 3. The proof follows from propositions 10 and 11. ■

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A The volume of B_0 containing a saddle point

A.1 The volume of B_0 in proposition 9

We first recall the definition of B_0. Let $\mathcal{O}$ be a neighbourhood as in proposition 5 such that f can be put into standard form c). Changing to cylinder coordinates (r,φ,s,ψ) and after an appropriate scaling we may assume that $f(r,\varphi,s,\psi) = r^2 - s^2$ and $B = \{(r,\varphi,s,\psi) \in \mathbb{R} \times S^{p-1} \times \mathbb{R} \times S^{q-1} \mid r+s \le 1\}$ is a subset of $\mathcal{O}$. Then we define $B_0 = \{(r,\varphi,s,\psi) \in B \mid 0 \le r^2 - s^2 \le h\}$ where $h \ge 0$. Now we wish to compute

$$\int_{B_0} 1\, d\xi\, d\eta = \int_{B_0} r^{p-1} s^{q-1} g_p(\phi) g_q(\psi) dr\, ds\, d\phi\, d\psi = c_{p,q} I_{p,q}(h).$$

The Jacobian of the transformation to cylinder coordinates is given by $r^{p-1}s^{q-1}g_p(\phi)g_q(\psi)$. The integrand does not depend on the angles so we split off the angular part and denote the integrals by a_p and a_q where a_m is the 'area' of the $m-1$ sphere. To facilitate the computations we make one further transformation: $u = r+s$, $v = r-s$. In the constant $c_{p,q}$ we absorb the constants a_p, a_q and the Jacobian of the change of coordinates (r,s) to (u,v). Furthermore we distinguish $h < 0$ and $h \ge 0$ and to simpify notation we write $k(u,v) = (u+v)^{p-1}(u-v)^{q-1}$. See figure 1 for the regions of integration.

$$I_{p,q}(h) = \begin{cases} I^-_{p,q}(h) = \int_{\sqrt{-h}}^1 \int_{-u}^{h/u} k(u,v) dv\, du, & h < 0 \\ I^+_{p,q}(h) = \int_0^1 \int_{-u}^0 k(u,v) dv\, du + \int_0^{\sqrt{h}} \int_0^u k(u,v) dv\, du + \int_{\sqrt{h}}^1 \int_0^{h/u} k(u,v) dv\, du, & h \ge 0 \end{cases}$$

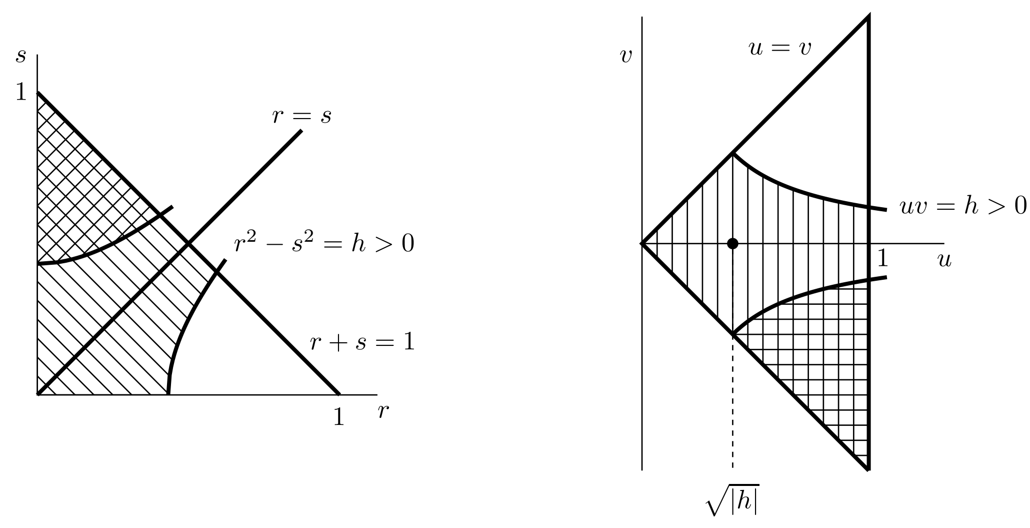

Figure 1: *Regions of integration for coordinates (r,s) and (u,v). Integral $I_{p,q}(h)$ for $h < 0$: doubly hatched region; $I_{p,q}(h)$ for $h \ge 0$: doubly and singly hatched region.*

After some computations it turns out that $I_{p,q}(h)$ consists of several parts: for both $h < 0$ and $h \ge 0$:

$$I^\pm_{p,q}(h) = P^\pm_{p,q}(h) \;+\; \alpha^\pm_{p,q}(\pm h)^{(p+q)/2} \;+\; \beta^\pm_{p,q}(\pm h)^{(p+q)/2} \log \sqrt{\pm h} \;+\; \gamma^\pm_{p,q}.$$

There is a constant part $\gamma^\pm_{p,q}$ because we consider the volume between levels -1 and h. This is done for computational reasons. Then continuity demands that $\gamma^+_{p,q} = \gamma^-_{p,q}$ which turns out to be true. Common to all cases is a polynomial part $P^\pm_{p,q}(h)$. The part with coefficient $\alpha^\pm_{p,q}$ may contain a square root depending on p and q and if the coefficient $\beta^\pm_{p,q}$ is nonzero there is a logarithmic part. The definitions of P, β, γ

and α are as follows

$$\begin{aligned}
P^+_{p,q}(h) = P^-_{p,q}(h) &= \sum_{k,m}{}^{(1)} \frac{\binom{p-1}{k}\binom{q-1}{m}(-1)^m h^{k+m+1}}{(k+m+1)(p+q-2(k+m+1))}, \\
\beta^+_{p,q} = \beta^-_{p,q} &= \sum_{k,m}{}^{(2)} \frac{\binom{p-1}{k}\binom{q-1}{m}(-1)^m}{(p+q)}, \\
\gamma^+_{p,q} = \gamma^-_{p,q} &= \sum_{k,m} \frac{\binom{p-1}{k}\binom{q-1}{m}(-1)^{p-1-k}}{(p+q)(p+q-(k+m+1))}, \\
\alpha^+_{p,q} = -\alpha^-_{q,p} &= \sum_{k,m}{}^{(1)} 2\frac{\binom{p-1}{k}\binom{q-1}{m}(-1)^m}{(p+q)(p+q-2(k+m+1))} + \sum_{k,m}{}^{(2)} 2\frac{\binom{p-1}{k}\binom{q-1}{m}(-1)^m}{(p+q)^2} \\
&= \frac{2}{(p+q)}\sigma_1(p,q) + \frac{2}{(p+q)^2}\sigma_2(p,q).
\end{aligned}$$

The sum $\sum^{(1)}_{k,m}$ is taken over all k and m satisfying $0 \le k \le p-1$, $0 \le m \le q-1$ and $2(k+m+1) \ne (p+q)$, whereas the sum $\sum^{(2)}_{k,m}$ is taken over the same range of k and m but now $2(k+m+1) = (p+q)$. The last line defines σ_1 and σ_2. With these definitions $\beta^+_{p,q} = \frac{2}{(p+q)}\sigma_2(p,q)$. The following properties of σ_1 and σ_2 are easily checked.

1. $\sigma_1(p,q) = (-1)^q\sigma_1(p,q)$, so $\sigma_1(p,q) = 0$ for q odd,
2. $\sigma_2(p,q) = (-1)^{q-1}\sigma_2(p,q)$, so $\sigma_2(p,q) = 0$ for q even,
3. $\sigma_2(p,q) \ne 0$ only if $p+q$ even, so using 2) $\sigma_2(p,q) \ne 0$ only if both p and q are odd.

Now the next lemma is immediate.

Lemma 12 *For each p and q the $\lceil \frac{n}{2} \rceil$-th derivative of $I_{p,q}$ as a function of h is discontinuous at $h = 0$. The nature of the discontinuity depends on p and q. For both p and q even it is a jump, for p and q odd the discontinuity is a log-like singularity and for $p+q$ odd it is a root-like singularity.*

A.2 The volume of B_0 in proposition 11

The computation of the volume of B_0 in proposition 11 is similar to that in section A.1. Here we only indicate the differences.

First note that p and q have a slightly different meaning because $p+q = n-1$. In this case the function k in the expression for $I_{p,q}(h)$ is given by $k(u,v) = (h-uv)(u+v)^{p-1}(u-v)^{q-1}$. With this definition of k the functions $I^\pm_{p,q}(h)$ are defined as before. Again after some computations we find

$$I^\pm_{p,q}(h) = P^\pm_{p,q}(h) + \alpha^\pm_{p,q}(\pm h)^{(p+q+2)/2} + \beta^\pm_{p,q}(\pm h)^{(p+q+2)/2}\log\sqrt{\pm h} + \gamma^\pm_{p,q} + \delta^\pm_{p,q}h.$$

The expressions for P, α, β and γ are more involved than in the previous section. Their structure, however, is similar therefore we skip the details. The relations are equal. There is one new term in the expression above which is defined as

$$\delta^+_{p,q} = \delta^-_{p,q} = \sum_{k,m} \frac{\binom{p-1}{k}\binom{q-1}{m}(-1)^{p-1-k}}{(p+q)(p+q-(k+m+1))}.$$

Thus we come to the same conclusion as in section A.1.

Lemma 13 *For each p and q the $\lceil \frac{n+1}{2} \rceil$-st derivative of $I_{p,q}$ as a function of h is discontinuous at $h = 0$. The nature of the discontinuity depends on p and q. For both p and q even it is a jump, for p and q odd the discontinuity is a log-like singularity and for $p+q$ odd it is a root-like singularity.*

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